THE ARTICLES ACCOMPANYING THIS FINAL REPORT
ARE REFERENCE MATERIAL FOR THE FINAL.
THE INVESTIGATOR MEANT ONLY TO INCLUDE FIRST PAGES

ARO 20616.14-EL

SEMICONDUCTOR HETEROSTRUCTURES AND NEW FORMS OF DEVICES

PROGRESS REPORT NO. 7
(FINAL)

K. HESS

SEPTEMBER 1986

U. S. ARMY RESEARCH OFFICE
ARO PROP. NUMBER: 20616-EL

DAAG 29-84-K-0001

COORDINATED SCIENCE LABORATORY
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN
URBANA, IL 61801

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) AD-A172 731

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: ARO 20616.14-EL	2. GOVT ACCESSION NO.: N/A
3. RECIPIENT'S CATALOG NUMBER: N/A	
4. TITLE (and Subtitle): Semiconductor Heterostructures and New Forms of Devices	5. TYPE OF REPORT & PERIOD COVERED: Final Report 1 Oct 83 - 31 Aug 86
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): K. Hess	8. CONTRACT OR GRANT NUMBER(s): DAAG 29-84-K-0001
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL 61801	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: N/A
11. CONTROLLING OFFICE NAME AND ADDRESS: U. S. Army Research Office, Post Office Box 12211, Research Triangle Park, NC 27709	12. REPORT DATE: September 1986
	13. NUMBER OF PAGES
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report): Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

The view, opinions, and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Superlattices
III-V Heterolayers
Heterlayer Transport
Heterolayer Devices

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The ultimate limitations of electronic transport in semiconductor hetero-structure layers and superlattices are investigated. The potential of these layers for novel semiconductor device applications is assessed.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

1. Brief Progress Summary and Discussions of Published Manuscripts.

We have investigated properties of III-V compound lattice matched heterolayers to explore their ultimate limitations and advantages for high speed semiconductor devices. During the past three years of this grant, twelve manuscripts (abstracts attached) were published or accepted for publication and eight invited presentations have been given. The three most significant achievements have been the development of:

(i) The first Monte Carlo simulation of the high electron mobility transistors (HEMT)

(ii) The first Monte Carlo model of planar doped barrier PDB transport including plasmon scattering and the Pauli principle, and

(iii) A new ultrafast switching device based on a combination of tunneling and hot electron thermionic emission.

Manuscript [1] summarizes high speed transport in submicron high electron mobility transistors (HEMT's). The manuscript deals mainly with the physical effects which are important for the HEMT operation and to a lesser extent with actual device performance.

The simulations show that significant velocity over-shoot exists in these structures and precise values of the over-shoot velocity are given. The device speed is substantially enhanced by this effect for devices of 1/2 micrometer feature sizes and below.

We have completed the simulation code for PDB's including standard transport effects as well as scattering by coupled phonon-plasmons, electron-electron pair interactions, ionized impurity scattering and also the Pauli principle.

The results of our calculations have been compared with experiments of Hayes and coworkers at AT&T Bell Laboratories and of Heiblum and coworkers at IBM.

We found that there is an overall agreement between theory and experiment (manuscript II) but the experimentally found energetic width (broadening) of the ballistic peak is much greater than predicted by the theory in the Hayes experiment and slightly greater in the experiment by

Heiblum et al. We attribute the broadening of the Hayes experiment to the fluctuating impurity potentials at the barriers (there are only a few impurities across the width of thin barriers). $GaAs-Al_xGa_{1-x}As$ heterolayers and therefore their barriers do not suffer from these fluctuations. The broadening in the experiments of Heiblum et al. can be attributed to electron-electron scattering. A report about the experimental work and our theory has appeared in Science (Vol. 231, p.22). Details are given in the attached manuscript.

Manuscript (III) demonstrates a new semiconductor switching phenomenon and infers from a phenomenological theory, switching times of $\geq$ 200 femtoseconds. We are especially excited about this project which could lead to an enormously fast semiconductor switching circuit element.

Perhaps the most complete study of interface electronic transport in (5) subbands at the AlGaAs-GaAs interface has been started by Yokoyama (manuscript IV, V) and is currently being completed by Artaki who also includes transport at low temperatures (4.2K).

Smaller projects have included time dependent ensemble Monte Carlo simulations for planar doped GaAs structures (manuscript VI) transport in superlattices including collision broadening (manuscript VII) and effects of size quantization on electrons and hole transport (Manuscript VIII and IX). While the latter papers are mainly devoted to the inclusion of quantum effects into otherwise semiclassical Monte Carlo simulations, we have also taken the first steps to a full quantum transport theory involving Feynman path integrals. The work which has been accomplished includes: Solutions of the linearly coupled electron-acoustic phonon system and comparison of results with analytic work and calculation of the density matrix and expectation values of electronic properties as a function of time.

Our experience in the projects outlined above has been summarized in two book chapters (manuscript X and XI) as well as in eight invited presentation (manuscript XII and list below).

2. Invited Presentations:

"Principles of Hot Electron Thermionic Emission (Real Space Transfer) in Semiconductor

Heterolayers and Device Applications", 1st Intern. Workshop on Future Electron Devices, Tokyo, February 1984.

"Transient Electron Transport in Semiconductor Heterolayers", Gordon Conference on MIS Systems, Tilton, NH, July 1984.

"Principles of Hot Electron Thermionic Emission (Real Space Transfer) in Semiconductor Heterolayers and Device Applications," European Physical Society 5th General Conference of the Condensed Matter Division of the EPS, Berlin (West), March 18-22, 1985.

"Electronic Transport in Semiconductor Heterolayers and Promising Device Concepts", Program of the 34th WEH-Seminar, Bad Honnef, May 13-15, 1985.

"Properties and Applications of Multiquantum Well and Superlattice Structures," American Vacuum Society 32nd National Symposium, Houston, TX, November 19-21, 1985.

"Analysis and Simulation of Semiconductor Devices," Scientific Applications and Algorithm Design for High Speed Computing Workshop, Urbana, IL, April 7-10, 1986.

"Computations of Electronic Transport in Semiconductor Heterolayer Structures." The First US-Japan Joint Workshop on Electronic/ Optoelectronics with Focus on "Optical Bistability, Optical Computation and Quantum Well Devices", Tokyo, Japan, May 28-30, 1986.

"Monte Carlo Simulations of Electronic Transport in Semiconductor Heterolayers," The Conference on the Forefronts of Large-Scale Computational Problems," Troy, NY 16-18, 1986.

3. Scientific Personnel:

K. Hess Professor

J. P. Leburton Assistant Professor

B. Mason Post Doctoral Research Associate

M. Artaki (Ph.D. student; Ph.D. final Oct. 1986)

T. Wang (Ph.D. student; Ph.D. completed 1985)

K. Brennan (Ph.D. student; Ph.D. completed 1984)

4. Interactions.

Much of the work has been performed in close cooperation with Dr. G. J. Iafrate, Ft. Monmouth.

Calculation of the electron velocity distribution in high electron mobility transistors using an ensemble Monte Carlo method

T. Wang and K. Hess
Department of Electrical Engineering, and the Coordinated Science Laboratory, University of Illinois, Urbana, Illinois 61801

(Received 25 January 1985; accepted for publication 6 February 1985)

The electron velocity distribution is calculated for an idealized model of the high electron mobility transistor using a many-particle Monte Carlo model and a self-consistent two-dimensional Poisson solver. Hot electron effects, nonstationary effects, and real space transfer are analyzed. The results show that significant velocity overshoot, 2.8×10^7 cm/s at 300 K and 3.7×10^7 cm/s at 77 K exists under the gate and that the velocity overshoot is limited by both k-space transfer and real-space transfer. The values of the overshoot velocities are much smaller than those obtained from the more conventional drift-diffusion model.

I. INTRODUCTION

In recent years, the high electron mobility transistor (HEMT) has attracted considerable interest because of its potential for ultrahigh-speed, low-power logic applications.[1-4] The key feature of the HEMT leading to its superior properties and distinguishing it from other field-effect transistors is the greatly enhanced electron velocity in the unintentionally doped GaAs channel. Currently, considerable theoretical and experimental effort is underway to determine the precise reasons for the speed advantage under high-field and transient conditions.[5-9] It has been demonstrated that the high switching speed of the HEMT is due to the following factors: (i) the high mobility in the source access region, (ii) overall quantum effects in the conducting channel, and (iii) significant nonstationary effects in the high-field range (velocity overshoot and ballistic transport).[8-10] Among these factors, the quantum effects have been recently investigated by Widiger *et al.*[8,9] and found to be of little consequence for electrons that are strongly heated by the drain field and hence cannot easily be confined to the interface potential well. The drift-diffusion model of Widiger *et al.*[8] is advantageous for describing the overall features of the HEMT. However, a more sophisticated approach based on the Boltzmann transport equation is needed to characterize the nonstationary phenomena which arise in the high-field region close to the drain contact. It is the purpose of this paper to present a many-particle Monte Carlo simulation including a complete band structure for both the GaAs and the AlGaAs layers as well as all relevant scattering mechanisms and a self-consistent two-dimensional solution of Poisson's equation. Our code appears to be well suited to explore the fundamental physics of hot electron transport in HEMT's, especially the effects of k space and real-space transfer[11] and velocity overshoot. We also study the effect of interelectronic collisions on the device performance.

Furthermore, a comparison between the drift-diffusion model and the Monte Carlo simulation is presented and the validity of the drift-diffusion equation in the high field region is examined by directly comparing overshoot velocities obtained from these two models.

II. METHOD OF ANALYSIS

A. Device geometry and boundary conditions

The device structure illustrated in Fig. 1 is used in all the simulations. The approximate vertical source and drain contacts used in the simulated structure generate virtually no difference compared to the planar ones in real devices since the potential drop in the regions directly under the source and drain is insignificant.[12] We have chosen a relatively low impurity concentration of 2×10^{17} cm^{-3} in the AlGaAs layer and in the n^+ contact regions to avoid complications arising from the Pauli exclusion principle. Although such a low doping level is unrealistic in real devices, it is of little consequence to the main subject of our study, the transport behavior of electrons in the high-field channel, because the carrier concentration in the high field region is always low.

Charge neutrality is assumed in the regions adjacent to the source and drain contacts throughout the entire simulation and serves as a boundary condition for the electron concentration. The boundary conditions for the electric potential which are used in the model are the Dirichlet condition (constant potential) at all metal-semiconductor surfaces and

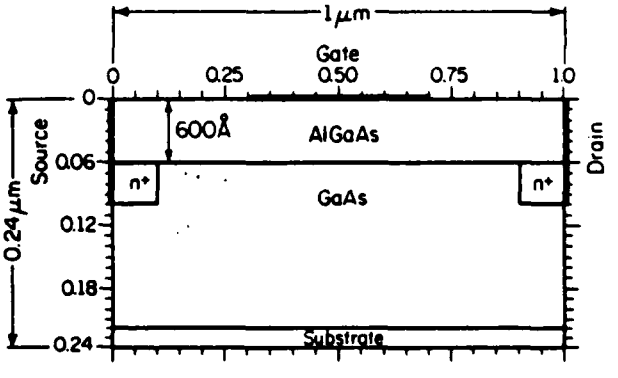

FIG. 1. Schematic representation of the computer simulation geometry of the AlGaAs-GaAs HEMT. The impurity concentration is 2×10^{17} cm^{-3} in the n-AlGaAs layer and in n^+ GaAs contact regions. The GaAs channel is unintentionally doped. An effective gate bias (including the Schottky barrier height) of -0.35 V is applied and the drain bias is 0.5 V.

 0021-8979/85/125336-04$02.40

Monte Carlo simulations of hot-electron spectroscopy in planar-doped barrier transistors

T. Wang and K. Hess
Department of Electrical Engineering and the Coordinated Science Laboratory, University of Illinois, Urbana, Illinois 61801

G. J. Iafrate
U. S. Army Electronics Technology and Devices Laboratory, Fort Monmouth, New Jersey 07703

(Received 4 November 1985; accepted for publication 27 November 1985)

We have developed a microscopic model to study the hot-electron-spectroscopy method which uses GaAs planar-doped barrier transistors. Our simulation is based on the Monte Carlo method and includes the effects of ionized impurity scattering, pair electron-electron scattering, long-range plasmon scattering, and coupled plasmon/phonon scattering. The nonparabolicity of the band structure and the Pauli exclusion principle are also taken into account in the highly doped base region. The numerical results show that the experimental method of Hayes will indeed reflect the overall momentum distribution of injected hot electrons if the planar-doped barriers are "ideal." Ideal means that the self-consistent potential (due to conduction electrons and ionized impurities) is well described by the continuum approximation. We demonstrate that potential fluctuations arising from the discrete natue of the charges and reflection of electrons at the base-collector junction make it impossible to obtain the precise distribution function from the experiments.

In recent years, extensive theoretical analyses have been performed[1-4] to assess the magnitude of velocity-overshoot effects and the possibility of the concept of ballistic transport.[5] Experimental verifications of the numerous theories have been rare and very indirect. The results of the Monte Carlo simulations of planar-doped barrier (PDB) devices by Hesto *et al.*[6] and Wang *et al.*[2] suggested the usefulness of PDBs for the investigation of ballistic transport phenomena.[7] In a series of papers, Hayes *et al.*[8-10] presented experimental results for the current voltage characteristics of planar-doped barrier transistors. They inferred that the electron-momentum distribution can be obtained by differentiating their measured current with respect to the collector voltage. Using this relation, they have been able to deduce important results for the electron mean-free time of flight, the velocity overshoot, and the fraction of ballistic (unscattered) electrons which travel through the transistor base.

The purpose of this paper is twofold. First, we develop a microscopic theory of transport in planar-doped barrier devices by using an ensemble Monte Carlo model which includes all known scattering mechanisms (including the electron interaction with coupled plasmon/phonon modes) as well as important quantum principles such as the Pauli principle, which is not usually included in these simulations. Second, we apply this first principle theory to the experiments of Hayes *et al.* in order to assess the accuracy of their evaluation of the distribution function. We find that overall, their experiments will resolve the distribution function if reflections at the collector barrier can be neglected. Also, potential fluctuations due to the discrete nature of impurities must be negligible if their conclusions on the scattering rate are to be correct.

In order to precisely simulate electron transport in devices having heavily doped regions, our current model includes the following features (in addition to the conventional mechanisms): (i) elastic-ionized-impurity scattering, (ii) long-range plasmon scattering in addition to short-range electron-electron scattering, (iii) coupled plasmon/phonon scattering, and (iv) the Pauli exclusion principle.

Since ionized impurity scattering and the pair electron-electron interaction are well known and have been described previously in connection with Monte Carlo methods[11,12], we concentrate here on the addition of the plasmon effect. Plasmons and coupled plasmon/phonon phenomena have been treated extensively in the literature.[10,13,14] Plasmons are due to the long-range Coulombic interaction between the electrons. They are typically of long wavelength and therefore all treatments known to the authors imply the extension of the electron gas over considerable distances. Naturally in ultrasmall devices these long distances may not be present. In fact, a base of 600 Å length doped with 10^{18}-cm^{-3} electrons will, on average, only contain six electrons over its length. These six electrons will not support plasmon oscillations of wavelength larger than the base width. There is also another natural limit of the plasmon wavelength λ as λ goes to zero.[13] This limit is usually taken to be twice the inverse of the Thomas–Fermi wave vector.[13] When calculating the electron plasmon/phonon interaction we therefore include these two limits, the device length (as $\lambda \to \infty$), and the Thomas–Fermi wave vector (as $\lambda \to 0$) in the integration of the scattering rate. The electrons still can interact in principle with the two-dimensional plasmons which propagate parallel to the emitter-base interface. However, the electrons entering the base have initially negligible momentum parallel to this interface. Also, as will be described later, we are mainly interested in forward momentum changes and therefore will ignore the coupling to the two-dimensional plasmons.

 0021-8979/86/062125-04$02.40

New Ultrafast Switching Mechanism in Semiconductor Heterostructures

K. Hess, T. K. Higman, M. A. Emanuel and J. J. Coleman

Center for Compound Semiconductor Microelectronics
Coordinated Science Laboratory
University of Illinois
1406 West Green Street
Urbana, Illinois 61801

(Received

Abstract

A new switching mechanism in a two-terminal semiconductor heterolayer structure is proposed which capitalizes on non-linear electron temperature effects in adjacent heterolayers. The estimated switching speed of an optimized heterostructure hot electron diode should be extremely fast, perhaps as fast as 200 femtoseconds. Data are presented on prototype devices which show the expected negative differential resistance and indicate that the basic physical model is correct.

Intersubband phonon overlap integrals for AlGaAs/GaAs single-well heterostructures

Kiyoyuki Yokoyama and Karl Hess
Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 1 March 1985)

The five lowest subband coupling coefficients $H_{mn}(Q)$ are calculated for polar-optical-phonon scattering in $Al_{0.3}Ga_{0.7}As/GaAs$ single-well heterostructures. The wave functions are calculated self-consistently within the effective-mass approximation including exchange and correlation effects.

Much effort has been made to advance the understanding of the electronic transport properties of quasi-two-dimensional systems.[1] Following the pioneering studies of Stern and Howard for inversion layers of metal-oxide semiconductor field-effect transitors (MOSFET's),[2] Ando performed detailed studies of MOSFET's and AlGaAs/GaAs single-well structures.[3] Simultaneously, lattice scattering for electrons in heterolayers has been extensively studied.[4-6] Intrasubband scattering is well understood. Intersubband scattering has been investigated in less detail.[6] It is the purpose of this Communication to present an accurate calculation of the overlap integrals which are necessary to determine intersubband scattering by phonons. The two-dimensional carrier scattering rate between mth and nth subbands is proportional to[5]

$$|M_{mn}|^2 = \int |Q,q)|^2 |I_{mn}(q)|^2 dq \ , \tag{1}$$

where $M(Q,q)$ is the corresponding three-dimensional matrix element, and Q and q are phonon-wave-vector components parallel (xy plane) and normal (z direction) to the layer interfaces, respectively. The overlap integral is expressed as[5]

$$I_{mn}(q) = \int F_m(z) F_n(z) \exp(iqz)\, dz \ , \tag{2}$$

where $F_m(z)$ is the normalized envelope function corresponding to the quantized energy of E_m.

Polar-optical-phonon scattering is one of the dominant scattering mechanisms above 77 K in III-V compound semiconductors. For polar-optical-phonon scattering, $|M(Q,q)|^2$ is proportional to $1/(Q^2+q^2)$. Accordingly, the scattering rate is proportional to $H_{mn}(Q)/Q$, where the multisubband coupling coefficients are expressed as[6]

$$H_{mn}(Q) = \int\int dz_1 dz_2 F_{mn}(z_1) F_{mn}(z_2) \exp(-Q|z_1 - z_2|) \ . \tag{3}$$

Here $F_{mn}(z) = F_m(z) F_n(z)$.

Since most of the electrons populate the lowest subband at low temperatures, the value of $H_{11}(Q)$ has been worked out in detail.[7] However, the electron occupation probability of higher subbands increases in high electric fields (the electrons become hot), and both intrasubband scattering in higher subbands and intersubband scattering among higher subbands are no longer negligible, even at a lattice temperature of 77 K. Under these conditions, the knowledge of the coefficients $H_{mn}(Q)$ is necessary in order to accurately calculate the optical phonon scattering rates for each subband. Self-consistent numerical calculations provide not only the quantized energy levels (E_m) but also the corresponding wave functions [$F_m(z)$] for a realistic AlGaAs/GaAs single-well heterostructure. Using these wave functions, accurate values of $H_{mn}(Q)$ can be obtained. The self-consistent calculation is briefly described in the following.

The normalized wave-function $F_m(z)$ for the mth subband can be obtained from the Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\frac{d^2F_m(z)}{dz^2} + V(z)F_m(z) = E_m F_m(z) \ . \tag{4}$$

The effective potential $V(z)$ is given by

$$V(z) = -e\phi(z) + V_h(z) + V_{xc}(z) \ , \tag{5}$$

where $\phi(z)$ is the electrostatic potential given by the solution of Eq. (6) below, $V_h(z)$ is the step function describing the interface barrier, and $V_{xc}(z)$ is the local exchange correlation potential.[8] We take into account the five lowest subbands. Then, Poisson's equation reads

$$\frac{d^2\phi(z)}{dz^2} = \frac{e}{\epsilon_0\epsilon}\left[\sum_{i=1}^{i=5} N_i F_i^2(z) + N_A(z) - N_D(z)\right] \ , \tag{6}$$

where N_i represents the number of electrons in subband i and is given by

$$N_i = \frac{m^* k_B T}{\pi\hbar^2} \ln\left[1 + \exp\left(\frac{E_F - E_i}{k_B T}\right)\right] \ . \tag{7}$$

$N_A(z)$ and $N_D(z)$ are the position-dependent acceptor and donor concentrations, and E_F is the Fermi energy.

In the calculation, we used an effective mass $m^* = 0.067 m_0$ and a dielectric constant $\epsilon = 13.0$ uniformly in both GaAs and AlGaAs. We have assumed abrupt interfaces, a barrier height of 0.3 eV, and we have neglected the image force term in Eq. (5). All of these approximations are very reasonable according to the results reported by Stern.[9] Moreover, the mobile charge in the AlGaAs layer was assumed to be depleted except for the penetration of the wave function of electrons from GaAs into AlGaAs. To solve the Schrödinger equation, we used the Numerov method,[10] which is efficient to obtain the pairs of eigenvalues and eigenfunctions accurately within short computational times.

Figure 1 shows the calculated effect potential according to Eq. (5) together with the five lowest subband energy levels at 77 K. The broken line indicates the electron concentration which is derived from the first term in the right parentheses of Eq. (6). The structure parameters are shown in the figure caption. The calculated energy differences

Monte Carlo study of electronic transport in $Al_{1-x}Ga_xAs/GaAs$ single-well heterostructures

Kiyoyuki Yokoyama and Karl Hess
Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 16 August 1985; revised manuscript received 3 March 1986)

A study of electronic transport in $Al_{1-x}Ga_xAs/GaAs$ single-well structures including multisubband conduction at 77 and 300 K has been performed. The electronic states of the quantum well are calculated self-consistently taking the five lowest subbands into account. The numerically obtained wave functions and energy levels are used to obtain the major two-dimensional scattering rates in each subband. Polar optical- and acoustic-phonon (via deformation-potential) scattering are considered including intersubband transitions. For ionized impurity scattering, the screening effects due to the five lowest subbands are taken into account to obtain the Fourier-transformed Coulomb potential. The steady-state and transient behavior of the electrons in the well are studied through a Monte Carlo particle simulation. It is shown that high transient velocities [$(3-8)\times 10^7$ cm/sec] can be expected at low and intermediate fields.

I. INTRODUCTION

Enhanced electron mobility in modulation-doped $Al_{1-x}Ga_xAs/GaAs$ heterostructures has been suggested by Esaki and Tsu[1] and demonstrated independently by Dingle, Störmer, Gossard, and Wiegmann.[2] Subsequently, much attention has been focused on modulation-doped heterostructures in order to realize ultra-high-speed field-effect devices, such as the high-electron-mobility transistor (HEMT).[3] Among some other combinations of III-V compound semiconductors, the largest effort has been devoted to study the $Al_{1-x}Ga_xAs/GaAs$ system.[4]

In this system, the $Al_{1-x}Ga_xAs$ layer is doped n type, while the adjacent GaAs layer is grown as pure as possible (*not intentionally doped*). The free electrons are transferred to the high-purity GaAs layer where they populate a narrow potential well and form a quasi-two-dimensional electron gas (Q2D EG). Since the electrons are spatially separated from the ionized donors, they exhibit a high-electron mobility even at high carrier densities. In fact, very impressive high-mobility values have been reported.[5-7] It has also been demonstrated that single period heterostructures exhibit better low-field mobilities than multiple heterolayers.[8]

Not only experimental but also theoretical work has been stimulated to understand electronic transport in heterolayers. Investigations of quasi-two-dimensional systems[9] have originally been performed for the inversion layers of metal-oxide-semiconductor field-effect transistors (MOSFET's). Following the pioneering studies of Stern and Howard for MOSFET's,[10] Ando carried out detailed calculations of MOSFET's and $Al_{1-x}Ga_xAs/GaAs$ single-well structures.[11] In these studies, the subband structure has been calculated using wave functions and energy levels which are obtained by a self-consistent calculation based upon the effective-mass approximation.

Simultaneously, lattice scattering[12-16] and impurity scattering[14,16-19] for electrons in heterolayers have been extensively investigated. Many of the above treatments have assumed square-well potentials and approximate wave functions to express the scattering rates analytically. Walukiewicz, Ruda, Lagowski, and Gatos[20] used a triangular-well approximation to discuss the electron mobility more realistically. For impurity scattering in Si inversion layers, Mori and Ando reported formulas using variational functions.[17] However, they focused their attention upon low temperatures to discuss the ultimate limits of the mobility values. Their final results are not applicable at high temperatures.

In all previous publications, the electron mobility values have been calculated from a relaxation time which is closely related to the inverse of the scattering rate. For device applications, we need to understand the warm- and/or hot-electron behavior of the quantum well system at and above 77 K. To study the transport properties in this regime, the Boltzmann transport equation must be solved taking into account the scattering in each subband of the $Al_{1-x}Ga_xAs/GaAs$ single-well potential. A Monte Carlo method[21] can bypass the difficulties in directly solving the complicated system of equations. Hot-electron velocity characteristics for a strictly two-dimensional system confined in a square well of $Al_{1-x}Ga_xAs/GaAs$ have already been studied previously using the Monte Carlo method.[22]

In this paper, we present more precise calculations of electron transport properties for $Al_{1-x}Ga_xAs/GaAs$ single-well heterostructures including multisubband conduction by means of an ensemble Monte Carlo method. In Sec. II, the electronic states of the quantum well are calculated self-consistently taking the five lowest subbands into account. The numerically obtained wave functions and energy levels are used to calculate the major two-dimensional scattering rates at 77 and 300 K in Sec. III. Polar optical-phonon scattering and acoustic-phonon scattering (via the deformation potential) are studied for each subband including intersubband transitions. For ionized impurity scattering, the screening effects due to the five lowest subbands are considered to calculate the

Time-dependent ensemble Monte Carlo simulation for planar-doped GaAs structures

T. Wang and K. Hess
University of Illinois, 1101 West Springfield Avenue, Coordinated Science Laboratory, Urbana, Illinois 61801

G. J. Iafrate
U. S. Army Electronics Technology and Devices Laboratory, Fort Monmouth, New Jersey 07703

(Received 16 January 1985; accepted for publication 11 February 1985)

A time-dependent ensemble Monte Carlo simulation has been developed which includes the computation of the self-consistent electric field and electron concentration. The Monte Carlo code is used to study transient and steady-state transport in planar-doped-barrier (PDB) GaAs diodes and transistors. Results are presented for the temporal and spatial evolution of electronic transport through the PDB. We show that (i) average velocities achievable with a PDB are significantly above the steady-state velocities by about a factor of 3, (ii) the rise time of the electric current in the PDB is in the subpicosecond range for diode length below 2000 Å, (iii) a pronounced displacement current dominates the transient electronics at onset of injection, and (iv) polar optical phonon absorption contributes significantly to the thermionic-emission current over the barriers.

I. INTRODUCTION

Ultrathin GaAs planar-doped structures have attracted considerable attention in recent years.[1] They provide an alternative to Schottky barriers due to their fast switching, mixing, and rectifying properties and are useful for hot-electron injection in connection with nonstationary transport in submicron devices. In the past, several theoretical analyses have been performed ranging from highly simplified closed-form analytical treatments[1-5] to complicated Monte Carlo simulations.[6] The earliest analytical treatment was presented by Malik,[1] who made use of the Richardson thermionic-emission theory. Kazarinov and Luryi analyzed the device operation by using the drift-diffusion model[2]; Cook replaced the assumption of a constant mobility with an energy-transport model[4] based on Stratton's formalism[7]; and Littlejohn *et al.* presented a Monte Carlo model with fixed potential to study velocity overshoot.[6] These studies have demonstrated that hot-electron effects, transient phenomena, and the self-consistency of the electric field are crucial in the operation of planar-doped-barrier devices. In this paper, we therefore have developed a Monte Carlo code to include all these features; in addition, we have included in our simulation the interactions of the electrons among themselves, although this interaction is of little significance for the structures analyzed in this paper. Using our Monte Carlo simulations, we demonstrate and analyze the significance of velocity overshoot and propose a novel structure which extends velocity overshoot over a submicron spatial scale.

II. METHOD OF ANALYSIS

A. Device structure

A planar-doped structure consists of single or multiple layers which are highly doped and sandwiched between intrinsic material. By controlling doping concentrations and positions of these layers, one can tailor the conduction band profile. Typical examples of planar-doped devices are n^+-i-p^+-i-n^+ diodes and hot-electron transistors.[8] A schematic band diagram for an n^+-i-p^+-i-n^+ diode is shown in Fig. 1. Notice that the sandwiched p^+ layer is thin enough to be totally depleted in equilibrium.

B. Monte Carlo model and boundary conditions

Our ensemble Monte Carlo method incorporates the Γ-L-X valleys of the GaAs conduction band and includes effects of nonparabolicity. Material parameters such as nonparabolicities, valley separations, and transverse and longitudinal effective masses are obtained from experimental results as available and from pseudopotential calculations.[9] The scattering mechanisms included are electron-

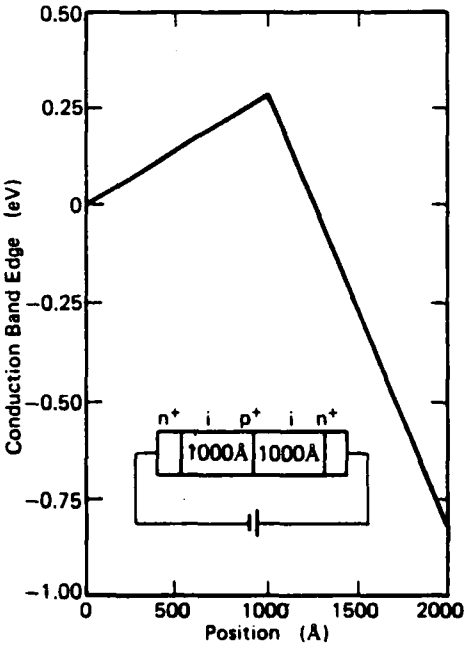

FIG. 1. Schematic representation of the band diagram of the n^+-i-p^+-i-n^+ structure shown in the inset of the figure with a bias voltage of 0.82 V. The area doping concentration in the p^+ plane is 1.0×10^{12} cm^{-2} and the volume concentration in the n^+ contact region is 1.0×10^{18} cm^{-3}.

 0021-8979/85/140857-05$02.40

MONTE CARLO CALCULATIONS OF ELECTRON TRANSPORT IN GaAs/AlGaAs SUPERLATTICES

Michael Artaki and Karl Hess

Coordinated Science Laboratory and
Department of Electrical and Computer Engineering
University of Illinois
Urbana, Illinois 61801

(Received 18 August 1985)

Electron transport in GaAs/AlGaAs superlattices was investigated by means of Monte Carlo simulations. The sources of scattering considered are acoustic and polar-optical phonons and ionized impurities. Collision broadening of the extended states is taken into account and its effect on the transport parameters is assessed.

I. Introduction

The concept of semiconductor superlattices has been introduced a few years ago by Esaki and Tsu [1] with the expectation that Bloch oscillations, a rather prohibitive phenomenon in bulk material, may really occur in such artificial structures. In superlattices, the artificial periodicity creates "mini" Brillouin zones with boundaries that can be reached by the electron before scattering to some other part of the zone.

The shape of the energy dispersion relation [1] shows that as the electron has the chance to cross the minizone it will reach a region where its mass becomes negative allowing for the observation of negative differential resistance.

The existence of Bloch oscillations and negative differential resistance has been predicted using the assumption of a constant scattering time [1,2] and also by Monte Carlo calculations [3,4] of the drift velocity when an electric field parallel to the growth axis of the superlattice is applied. These calculations have been performed by assuming that the electrons populate only the first superlattice subband and that the scattering agents are acoustic and polar optical phonons.

It is the purpose of this paper to investigate the influence of collision broadening on superlattice transport. The reason for our investigation is the small energy-width of the superlattice subbands (< 50meV). We therefore simulated steady state transport in a superlattice by going beyond the semiclassical Boltzmann equation along lines previously used by Chang et al [6].

We also include as an additional scattering mechanism of our simulation ionized impurity scattering.

II. Model of the Superlattice Studied

Our model is an idealization of a GaAs-$Al_xGa_{1-x}As$ superlattice having a mole fraction of $x \leq 0.3$. Given low x-values and the rather low values of the applied field it was assumed, as done by previous authors[3,4] that the electrons will not transfer to the subsidiary L and X minimum of GaAs or $Al_xGa_{1-x}As$.

The energy dispersion relation can therefore be approximated by:

$$E(\mathbf{k}) = E_n + \frac{1}{2}(-1)^n \Delta E_n \cos k_z d + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2) \qquad (1)$$

where the superlattice growth direction is the z-axis. (E_n is the center energy of the nth subband and ΔE_n its width.)

In determining the values of E_n and ΔE_n, we used the approach of Leburton and Kahen [7]. Their method is an extension of a simple Kronig-Penney periodic potential to account for some details of a more realistic electron structure. Using their results for a superlattice with $x = 0.1$, L_W (well width) = L_B (barrier width) = $8a_0$ (a_0 being the GaAs lattice constant) and assuming a 0.65/0.35 rule for the band edge discontinuity of the conduction and valence bands, we obtain:

$E_1 = 0.0721$ eV $\quad \Delta E_1 = 0.01726$ eV

$E_2 = 0.2199$ eV $\quad \Delta E_2 = 0.0551$ eV

The forbidden zone between the first and second subband is then 0.1289 eV.

III. Simulation method

The transport parameters were calculated with the standard one electron steady-state Monte Carlo simulation whose details have been described in detail by many authors (see for example Fawcett et al. [5]). The electron was launched at the bottom of the miniband and its trajectory monitored in the first superlattice minizone. Flight times and the types of scattering mechanisms ending the electron drift were determined stochastically according to the scattering probabilities.

0749-6036/85/060489+05 $02.00/0

Monte Carlo investigation of transient hole transport in GaAs

K. Brennan and K. Hess
Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

G. J. Iafrate
U.S. Army Electronics Technology and Devices Laboratory, Fort Monmouth, New Jersey 07703

(Received 14 December 1983; accepted for publication 26 January 1984)

Transient transport of holes in GaAs is studied under the conditions of high energy injection. This study is made using a Monte Carlo simulation with the unique inclusion of a realistic band structure based on the $K \cdot P$ method. The results reported herein show that a significant velocity overshoot occurs at low applied electric fields over distances greater than 1500 Å. As the applied field increases, the effect of the overshoot upon the transit time becomes less pronounced. There is no discernable gain in the drift velocity for holes injected at high energy, 0.1 eV, as compared to holes injected at zero launching energy for the distances considered here.

PACS numbers: 72.20.Js

Much attention has been focused recently upon developing high speed devices based upon velocity overshoot.[1-5] As originally proposed by Ruch,[6] use of velocity overshoot of electrons in GaAs and other III-V compounds can give a significant increase in carrier velocity over the steady-state value. The recent work of Tang and Hess[7] and Brennan *et al.*[8] has shown that there exists a limited set of conditions, the collision free window, under which velocity overshoot can be appreciable for electrons in GaAs and InP. However, the distances over which velocity overshoot persists have been found to be small.[7,8] There may be ways of artificially lengthening the range over which velocity overshoot can be attained. One method suggests that repeated overshoot can be achieved with electrons in GaAs through the use of potential steps.[9,10] The recent work of Brennan and Hess[10] shows that velocity overshoot of electrons can be maintained over distances of 0.5 μ or more by use of staircase structures.

Ruch found that the electron velocity overshoots its saturation value in both silicon and gallium arsenide.[6] However, the velocity overshoot persists an order of magnitude longer in GaAs than in Si due in part to the much faster energy relaxation in Si at low energies. The electron drift velocity also is substantially higher in GaAs than in Si at low applied fields[11,12] because of the different effective masses of the elecrons in each material. In GaAs, polar optical scattering is the dominant energy relaxation mechanism which on average is weaker than the deformation potential scattering present in Si. Therefore, it takes longer for the electron overshoot to relax in GaAs than in Si, leading to much higher electron drift velocities over longer distances.[7]

The presence of heavy holes and deformation potential scattering in the valence band of GaAs at low energy greatly diminishes the hole velocities. Therefore, one would expect that velocity overshoot of holes would be limited by the strong energy relaxation much as it is in silicon. However, our calculations show that the velocity overshoot of holes in GaAs is significant under certain conditions of field and launching energy. Velocity overshoot of holes in GaAs is not as pronounced as that of electrons in GaAs but it is larger than for electrons in silicon, as calculated by Ruch.[6]

Our calculations are performed using a Monte Carlo program with a realistic valence band structure[13] based on a $K \cdot P$ calculation.[14] It is essential that a realistic band structure be used because the valence bands are strongly warped and nonparabolic even at low energy.[15] We include the split-off band as well as the heavy and light hole bands in the calculation. The hole-phonon scattering rate is determined using a field theoretic approach[16,17] and is based on the total density of states present in all the bands. The probability of a hole transfering from one band to another via interband scattering is determined by directly calculating the overlap integrals.[15]

The predominant scattering mechanisms are polar optical and deformation potential scattering.[18,19] The principal scattering agents are acoustic, nonpolar, and polar optical phonons. The acoustic scattering rate is calculated using the method of Canali *et al.*,[20] and the value of the acoustic phonon coupling constant E_1^2 is determined from the work of Costato and Reggiani.[18] The value of the deformation potential constants "a, b, d," which are used in determining E_1^2, are taken from Wiley.[21] The transition probabilities for nonpolar optical scattering can be written in a manner that is completely analogous to that for acoustic phonon scattering[22] containing the optical deformation potential constant d_0. However, it is useful to express the nonpolar optical scattering rate in terms of the optical phonon coupling constant $(DK)^2$. $(DK)^2$ can easily be determined from E_1^2.[21] All of the parameters used in determining the hole-phonon scattering rate will be collected in a future publication.[23]

The overall scattering rate is calculated using both the results of Costato and Reggiani[18,19] and a field theoretic approach.[16,17] At low energy, the total phonon scattering rate is calculated from the sum of the acoustic, nonpolar, and polar optical scattering rates as determined by Costato and Reggiani.[18,19] Above approximately an energy of 0.5 eV, the total scattering rate is calculated based on the total density of states of all three valence bands. This rate is adjusted to match the low energy scattering rate at 0.5 eV. In the calculations presented here, the self-energy effects are significant at high applied fields: 100 and 200 kV/cm.

 0021-8979/84/103632-04$02.40

Size effects on polar optical phonon scattering of 1-D and 2-D electron gas in synthetic semiconductors

J. P. Leburton
Coordinated Science Laboratory and Department of Electrical Engineering, University of Illinois, Urbana, Illinois 61801

(Received 6 April 1984; accepted for publication 15 May 1984)

The total scattering rate and the transition probability for electron-phonon interaction in 1-D and 2-D semiconductor materials are calculated in taking into account the finite dimensions of the structure. Although noticeable, size effects on the scattering rate are generally small, with more pronounced features for 1-D structures than for 2-D structures. For 2-D layers, our theory agrees with recent experimental results whereas it contradicts the previous theory predicting large size effects and mass-independent electron-phonon scattering rates. In 1-D structures singularities in the phonon emission rate appear as a natural consequence of the 1-D density of states. However, for high energy the 1-D emission rate is found smaller than the corresponding 3-D rate. An additional consequence of the confinement is the quenching of the phonon absorption rate.

I. INTRODUCTION

The remarkable developments of fine line lithography and the new epitaxial technologies of molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD) have added astonishing possibilities to the fabrication of new artificial materials. Alternating structures of lattice matched III-V semiconductor compounds, as for example $Al_xGa_{1-x}As$ are presently fabricated with typical thicknesses of 10 nm or less and with accurately controlled doping. In these artificial materials, the layer dimensions are comparable to the de Broglie wavelength λ_e and the electrons are confined in the ultrafine structure. Transport is essentially two dimensional (2-D) and presents new characteristics not exhibited in bulk semiconductors. For example, the mobility parallel to the plane of the layer has been shown to be improved drastically by modulation doping of the structures and values as high as 10^6 cm^2/V s have been achieved.[1] Recently, an alternative structure based on the confinement of electrons in a "wire" semiconductor has been proposed to improve further the conducting properties of the materials.[2] In these one-dimensional (1-D) III-V synthetic materials, the electron gas is quantized in two transverse directions and the charge carriers can only move in the longitudinal direction. GaAs-AlAs quantum well wires have already been realized by Petroff *et al.*[3] and other structures based on field effects promise to be feasible in the near future.[4,5]

Because of the limited number of available final states during the scattering process (forward or backward scattering), the 1-D electron mobility is seemingly enhanced and its value has been estimated to be far beyond 10^6 cm^2/V s.[6] The obvious potential of these new structures for high-speed devices makes the knowledge of their transport parameters desirable. Although transport theory in 1-D semiconductor structures is still in its infancy, calculations of the most common scattering mechanisms impurity,[6-7] acoustical phonon,[8] and optical phonon[9] have already been performed. However, interaction with polar optical phonons (POP) merits special attention; the large energy exchange between carriers and lattice vibrations influences considerably transport at room temperature. Moreover, the POP interaction is a major scattering mechanism responsible for hot electron effects.[10] So far, the dependence of the POP scattering on the "wire" cross section has not been investigated. Yet, wire parameters appear to be technologically controllable, and owing to device applications, it is of importance to appreciate realistically the confinement effects on the electron-POP interaction. In this paper we derive the total POP scattering rate in 1-D semiconductor structures and discuss the influence of size effects on the electron-phonon interaction. Furthermore, we reconsider the corresponding 2-D transition probability. 2-D electron-POP interaction represents an important limitation on the high-speed performance of High Electron Mobility Transistor (HEMT). Although experimental data show a weakening of the electron-phonon interaction in 2-D structures compared to 3-D materials[11,12] theoretical models predict a larger scattering rate.[13] This discrepancy has been attributed to the screening of the electron-POP interaction by high-density carriers in 2-D structures. However, we believe that the discrepancy is partially due to crude approximations previously used for the 2-D calculation, e.g., $q_zL_z \ll 1$ (strictly 2-D gas), where q_z is the transverse component of the phonon wave vector and L_z is the layer width.[14,15] Hence, Ridley, introducing the momentum-conservation approximation (MCA) has obtained an expression for the 2-D scattering rate which is mass independent and varies as $1/L_z$.[16] Prior to these results, Price obtained a $\sqrt{m}$ law for the 2-D collision rate, the same as for 3-D electron gases.[17] He also has shown that the size effects are weaker than predicted by Ridley. In the following, we clarify this question by calculating exactly the phonon scattering rate for 2-D electron gases. Our theory generally agrees with experimental data from Chiu *et al.*[12] and shows that size effects lower the POP scattering rate. Screening effects, however, are not considered here and likely account for further lowering of the electron-POP interaction as claimed by Shah *et al.*[11] For 1-D electron gas, size effects are shown to have important consequences on the POP emission rate.

 0021-8979/84/222850-06$02.40

HIGH SPEED TRANSPORT IN ULTRASMALL DIMENSIONS

G. J. Iafrate

US Army Electronics Technology and
Devices Laboratory (ERADCOM)
Fort Monmouth, NJ 07703

K. Hess

Department of Electrical Engineering
and Coordinated Science Laboratory
1101 W. Springfield, Urbana, IL 61801

MODERN ASPECTS OF HETEROJUNCTION TRANSPORT THEORY

K. Hess
Department of Electrical and
Computer Science and the
Coordinated Science Laboratory
University of Illinois
Urbana, IL 61801

and

G. J. Iafrate
U.S. Army Electronics Technology
and Devices Laboratory
Fort Monmouth, NJ 07703

Festkörperprobleme XXV (1985)

Principles of Hot Electron Thermionic Emission (Real Space Transfer) in Semiconductor Heterolayers and Device Applications

K. Hess

Department of Electrical Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

Summary: The principles of real space transfer and its phenomenological description in terms of the concepts of electron temperature and quasi Fermi levels are reviewed. It is shown that real space transfer is a mechanism to achieve ultrafast switching and storage of charge carriers. The real space transfer-glow cathod analogy, which demonstrates the existence of a new transistor principle, is discussed in detail.

Introduction

The technologies of molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD) have opened a world of possibilities to create new forms of III–V semiconductor heterolayer materials. Structures hundred times as sophisticated and small as the smallest feature sizes in current silicon technology can be fabricated with ease. This fine tuned variability of structure and boundary conditions offers many opportunities for the development of new device concepts and research in this area is rapidly expanding [1].

Advantages of III–V compounds with respect to steady state mobility and transient electronic transport [1] (velocity overshoot) have long been known. However, the realization of these advantages in applications have been impeded by technological difficulties. MBE and MOCVD have provided a quantum leap in material quality and controlability, which together with the ideas of selective (modulation) doping [2] and achievable abruptness of heterointerfaces have increased the mobility values and potential device speeds by an order of magnitude. Studies of modulation doping have resulted in successful designs of the high electron mobility transistor [3] which draws its major advantage from the low source access resistance.

Simultaneously to these developments several other new effects, peculiar to the boundary conditions of complicated heterolayer structures, have been discovered. Examples are quantum well lasers [4], and real space transfer devices [5, 6]. It is the purpose of this paper to describe the physical basis of real space transfer and its